

STATEMENT

ADSORPTION / DESORPTION

OF

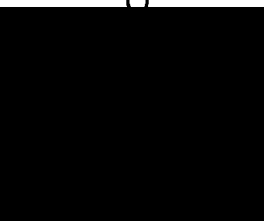


Date: 24 July 2002

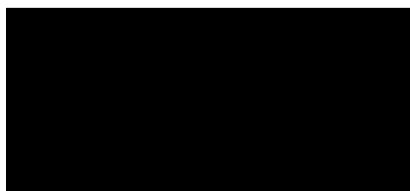
**NOTOX Project 338669
NOTOX Substance 111834**

Expert statement**Calculation of Adsorption/Desorption of**

The adsorption/desorption of has been calculated using the method described in the Technical Guidance Document on Risk Assessment (1996).



Structural Formula of the main component



Structural Formula of the minor component

Physical Chemical Data:

- Boiling temperature : Project no. 338568: Reaction or decomposition of the test substance was observed above 80°C. Boiling of the test substance was not observed below the temperature at which reaction or decomposition started.
- Density : Project no. 338579: 1.16 g/cm³ (20.0 ± 0.5°C).
- Vapour pressure : Project no. 338581: 761 ± 30 Pa Pa (20°C).
- Surface tension : Project no. 338592: 52.6 mN/m (20 ± 0.5°C).
- Water solubility : Project no. 338603: Test temperature: 20.0 ± 0.4°C at pH 3.5.
 During the test formed as a result of the reaction of the other
 was determined to be ≥ 230 g/l.
 the water solubility of was estimated to be ≥ 201 g/l.
 Based on
 Based on
 g/l.
 The water solubility of is given in the literature as 4000 ± 60 mg/l at 25°C.
- Partition coefficient : Project no. 338614: The results of the Estimation method and the Flask-shaking method were not in agreement.
 Results using the HPLC method:

The P_{ow} value for the major component in [REDACTED] is 3.60×10^1 ($\log P_{ow} = 1.6$) at $24.5 \pm 1.0^\circ\text{C}$.

The P_{ow} values for five minor components in [REDACTED] are values of 0.27, 0.85, 2.1, 3.2 and 3.4) at $24.5 \pm 1.0^\circ\text{C}$.

The adsorption/desorption of [REDACTED] is based on the major component [REDACTED] and the minor component [REDACTED] other water solubilities and correspondingly lower $\log P_{ow}$'s and are therefore of lesser concern.

Several chemical classes can be used:

Non Hydrophobics (I) and esters (II) having different QSAR's and a $\log P_{ow}$ of 1.6 (major component) has been used:

- (I) $\log K_{oc} = 0.52 \log P_{ow} + 1.02 = 1.85$
- (II) $\log K_{oc} = 0.49 \log P_{ow} + 1.05 = 1.83$

Mean Log Koc = 1.8 (range 1.83 – 1.85, based on the Log Kow of DMP).

Non Hydrophobics (I) and alcohols (II) having different QSAR's and a $\log P_{ow}$ of 3.2 and 3.4 (Isomers of the minor component) has been used:

- (I) $\log K_{oc} = 0.52 \log P_{ow} + 1.02 = 2.68$ ($\log P_{ow}=3.2$)
- (I) $\log K_{oc} = 0.52 \log P_{ow} + 1.02 = 2.79$ ($\log P_{ow}=3.4$)
- (II) $\log K_{oc} = 0.39 \log P_{ow} + 0.50 = 1.75$ ($\log P_{ow}=3.2$)
- (II) $\log K_{oc} = 0.39 \log P_{ow} + 0.50 = 1.83$ ($\log P_{ow}=3.4$)

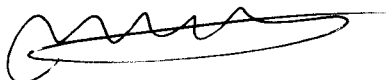
Mean Log Koc = 2.21 (range 1.75 – 2.68, based on the Log Kow = 3.2 of [REDACTED]).

Conclusion: The different QSAR's give different outcomes of the Log Koc. For risk assessment purposes in the European Economic Area, these calculated values should be used, in view of all uncertainties using QSAR.

For the main component [REDACTED]: Log Koc=1.84.

For the minor component [REDACTED] based on the two isomers: Log Koc=2.2 and Log Koc=2.3.

NOTOX B.V.



[REDACTED]
Assistant Registration Manager
(Industrial Chemicals)

CERTIFICATE OF ANALYSIS

Certificate of AnalysisTNA-2001007
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ICS-331

Product name :
Chemical name :
Batch number : 1510-14

Test results:

Method	Analysis of	Unit	Result * ¹
Jo/72.11, Jo/95.2	 <i>See page 2 for a specification</i>	% m/m	28.6 (± 1.5)
J20010792			
	e	% m/m	2.0 (± 0.3)
Amp/88.9	Water	% m/m	2.6 (± 0.3)
J20010792	Unidentified impurities	% m/m	0.5 (± 0.2)

*¹ bracketed values are estimated 95% confidence intervals

File code : TNA-2001007

Analytical documentation : 20010792

Authorized by

Name :
Function : Section Head, Analytical Research Department
Date : October 25, 2001

Signature :



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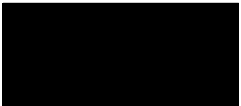






Certificate of Analysis



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structure	% m/m
<div></div> (Type IV) I 	18.6
<div></div> (Type III) I 	7.9
	2.1

P  ds